Problem II: Generalities

(a)

In a region of space, a particle with mass m and with zero energy (E=0) has a time-independent wave function:

$$\psi(x) = Axe^{-\frac{x^2}{L^2}} \tag{1}$$

where A and L are constants. Determine the potential energy U(x) of the particle. Remember that $\psi(x)$ is the solution of the Schrodinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi = E\psi \tag{2}$$

(b)

An electron is described by the wavefunction:

$$\psi(x) = \begin{cases} 0 & \text{for } x < 0 \\ Ce^{-x}(1 - e^{-x}) & \text{for } x > 0 \end{cases} \tag{3}$$

where x is in nm and C is a constant.

- Determine the value of C that normalizes $\psi(x)$.
- Where is the electron most likely to be found. That is for what value x is the probability of finding the electron maximal.
- Calculate the average position $\langle x \rangle$ for the electron. Compare the result with the most likely position. Comment.

  Hint: You could use the relation: $\displaystyle\int_0^\infty xe^{-ax}dx = \frac{1}{a^2}$

Problem III: The square well

Throughout this problem you can make use of the following relations:

$$\sin(2x) = 2\sin(x)\cos(x) \qquad \sin^2(x) = \frac{1 - \cos(2x)}{2} \qquad \cos^2(x) = \frac{1 + \cos(2x)}{2}$$

$$\sin(a)sin(b) = \frac{1}{2}\left[\cos(a - b) - \cos(a + b)\right]$$

$$\cos(a)\sin(b) = \frac{1}{2}\left[\sin(a - b) + \sin(a + b)\right]$$

, and integration by part:

$$\int x^n \sin(ax)dx = \frac{-x^n\cos(ax)}{a} + \frac{n}{a}\int x^{n-1}\cos(ax)$$

$$\int x^n \cos(ax)dx = \frac{x^n\sin(ax)}{a} - \frac{n}{a}\int x^{n-1}\sin(ax)$$

(a)

Determine the energy levels E_n and the normalized wavefunctions ψ_n of a particle in an infinite 'potential well'. The potential energy of the particle is:

$$V(x) = \begin{cases} +\infty, & \text{if } x < 0 \text{ or } x > a. \\ 0, & \text{otherwise.} \end{cases} \tag{4}$$

(b)

Prove that the determined wavefunctions $\psi_n(x)$ are orthonormal, that is:

$$\langle \psi_n | \psi_m \rangle = \int_0^a \psi_n^*(x)\psi_m(x)dx = \begin{cases} 1 & \text{if } m = n \\ 0 & \text{if m} \neq \text{n} \end{cases} \tag{5}$$

(c)

Show that for particles in a 'potential well', the following relations hold:

$$\langle x \rangle_{\psi_n} = \langle \psi_n | \hat{x} | \psi_n \rangle = \frac{a}{2} \tag{6}$$

$$\sigma_x^2|_{\psi_n} = \overline{(x - \langle x \rangle)^2} = \langle \psi_n | (x - \langle x \rangle)^2 | \psi_n \rangle = \langle x^2 \rangle - \langle x \rangle^2 = \frac{a}{12}(1 - \frac{6}{n^2\pi^2}) \tag{7}$$

Show that for large values of n, the above results agree with the classical result.

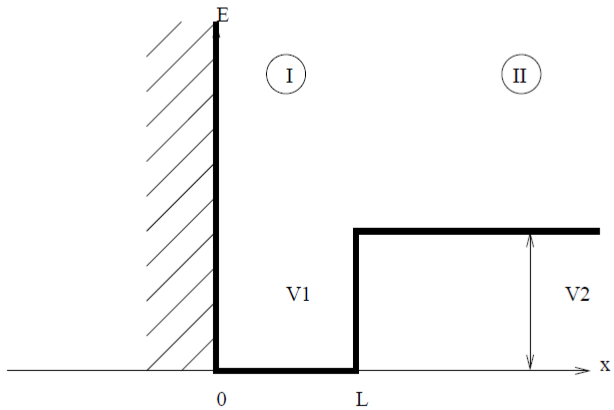
(d)

A particle in an infinite well is described by the wavefunction:

$$|\Psi\rangle = N\left((3 + 2i)|\psi_1\rangle - 2|\psi_2\rangle + 3i|\psi_3\rangle\right) \tag{8}$$

- Find N so that $|\Psi\rangle$ is normalized.
- What is the probability of finding the particle in states: $|\psi_1\rangle$, $|\psi_2\rangle$ and $|\psi_3\rangle$ respectively.
- What is the probability to find the particle in the region defined by: $\frac{a}{4} \leq x \leq \frac{3a}{4}$
- Find the mean value of the energy $\overline{E}$ in state Ψ
- Find the mean value of $\hat{p}$ in eigenstate ψ_n, and deduce its value in state $|\Psi\rangle$. The expression of operator $\hat{p}$ is given by $\hat{p} = -i\hbar\frac{d}{dx}$.
- Suppose we measure the state of the system at $t = 0$ and we obtain $|\psi_1\rangle$, which state would the particle occupy at later times ?

Figure 1: Asymmetric one-dimensional potential well.



(e)

A particle of mass m is subject to the 'asymmetric well' potential, shown in figure 1. We are interested by the energy levels $E > 0$ of the particle.

1. Evaluate the expression of the wavefunction in regions I) and II). For region II), one has to distinguish two cases: $E > V_2$ and $E < V_2$).
2. In order to obtain a bound state, what condition should be satisfied by the energy E ?
3. Let us consider the case of a bound state.
   - What condition should the wavefunction satisfy at 0 and $+\infty$.
   - Write the continuity condition of the wavefunction at $x = L$.
   - Deduce the equation giving rise to the energy levels quantization (without solving the equation).

Problem IV: State of an ammonia molecule

We consider an ammonia molecule and we restrict ourselves to the subspace E_0 formed by the linear combinations of the lowest energy states $|\psi_s\rangle$ and $|\psi_a\rangle$. In the basis $\{|\psi_s\rangle, |\psi_a\rangle\}$ the hamiltonian of the molecule is:

$$\hat{H} = \begin{pmatrix} E_0 - A & 0 \\ 0 & E_0 + A \end{pmatrix} \tag{9}$$

We define the operator $\hat{X}$ associated with the "disposition with respect to the center" X:

$$\hat{X} = d \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{10}$$

where d is a fixed, known parameter. A physical or chemical process (that we will not describe) produces the molecules always in the state:

$$|\psi(0)\rangle = cos\theta \, |\psi_s\rangle + sin\theta e^{i\phi} \, |\psi_a\rangle \tag{11}$$

with $0 < \theta < \frac{\pi}{2}$ and $0 < \phi < 2\pi$. We are looking for an experimental procedure which allows to determine these two parameters with a good precision. For this purpose we take 3N ammonia molecules ($N >> 1$) all prepared in the state $|\psi_0\rangle$.

(a)

For N molecules among the 3N available, we perform an energy measurement at time t = 0.

1. Prove that state $|\psi_0\rangle$ is normalized.
2. Calculate $\langle E \rangle$ for the state $|\psi_0\rangle$.
3. What are the possible results for an individual energy measurement?
4. Give the probability for each result and re-obtain the value obtained for $\langle E \rangle$.
5. What is the information one obtains on the unknown parameters θ and ϕ.

(b)

For N molecules among the remaining 2N, we perform a measurement of X at time t = 0.

1. What are the possible results in a measurement of X ?
2. Calculate the average value $\langle \hat{X} \rangle_0$ of the results for the state $|\psi_0\rangle$.
3. What is the complementary information that one obtains on the two unknown parameters θ and ϕ ? Is it now possible to determine unambiguously these two parameters ?

(c)

We let the N remaining molecules undergo a free evolution for a duration T, and we then perform a measurement of X on each of these molecules.

1. Write the state $|\psi(T)\rangle$ of these molecules just before the measurement of X.
2. Let T be such that $\frac{AT}{\hbar} = \frac{\pi}{4}$. Calculate the average value $\langle X \rangle_T$ of the results for the state $|\psi(T)\rangle$.
3. Show that the initially unknown state $|\psi_0\rangle$ is now fully determined if one combines the results of the three sets of measurements.